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Variational scattering theory using a functional of fractional form. II. An L^2 approach

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An L^2 approach to our variational method which is based on a functional of fractional form is proposed. As in the R-matrix theory, configuration space is divided into two parts. However, unlike the R-matrix theory, the associated wave function is always smooth. The resulting K matrix is anomaly-free and symmetric (and hence the S matrix is unitary). Application of this method to an exactly soluble two-channel model problem shows that our new approach gives much better results than the other standard variational principles.

I. INTRODUCTION

In an earlier paper (referred to as I.),[1] we proposed a new variational principle in which the variational functional is of a fractional form. In this variational functional the trial scattering wave function is not required to have the correct asymptotic form. In this paper, we will present an L^2-approach[2] to this new variational principle.

We have recently applied the Schwinger variational principle[3] to an exactly soluble two-channel model problem in order to compare it with other standard variational principles such as the anomaly-free[4] (AF), minimum-norm[5] (MN), optimized anomaly-free[6] (OAF), and restricted interpolated anomaly-free[7] (RIAF) methods. We found that the schwinger method gave results which were superior to those of the other variational methods. One of the important reasons for this is that since the trial wave function in the Schwinger principle is always associated with the potential function it must be expanded only over the region where the potential is nonzero.[8] On the other hand, in the standard variational principles the wave functions are expanded over the entire space. It is obvious that more basis functions are required if the wave function must be expanded over a larger region of configuration space. In fact, application of the Kohn variational principle by Rountree *et al.*[9(a)] and Collins *et al.*[9(b)] attempts to reduce the region of space which must be spanned by the square-integrable basis functions.

R-matrix theory attempts to partition configuration space as efficiently as possible.[10] Configuration space is divided into two parts, one of which is the strong potential region (interior region) and the other the zero (or very weak) potential region (exterior region). The interior and exterior regions are investigated using different methods and the wave functions in the two regions are matched on the boundary. However, in many approaches to the R-matrix theory, the logarithmic derivative can be discontinuous across the boundary and hence the resultant wave function is not necessarily smooth at this boundary.[11] To cope with this situation, various methods have been proposed.[11] However, Shimamura still concludes that no methods have yet been proposed which give both a continuous logarithmic derivative (i.e., smoothness) and a completely unitary S matrix.[11]

In this paper, we will present a method in which configuration space is divided just as in R-matrix theory. In our scheme this division of space also comes about naturally because the trial wave function is not required to have the correct asymptotic form. Owing to the form of the variational functional,[1] the resultant K matrix is symmetric (the S matrix is unitary) and also stationary. Furthermore, the wave function is completely smooth at the boundary. In Sec. II we will present the theory of this approach. The method is applied to an exactly soluble two-channel problem in Sec. III. The results are extremely encouraging.

II. THEORY

For simplicity, we will discuss only a single-channel version of the theory. Extension to the multichannel case is easy and straightforward.[1] Let us consider a radial scattering equation (in units of $m=\hbar=e=1$)

$$\left(E+\frac{1}{2}\frac{d^2}{dr^2}-V_L-V_S\right)\Psi=0\,, \tag{2.1}$$

where V_L is a long-range potential such as the Coulomb potential, and V_S a short-range potential such as Yukawa potential or exchange potential. Beyond some point B, V_S is assumed to be zero or negligible. We define a zeroth-order Hamiltonian H_0 as

$$H_0=-\frac{1}{2}\frac{d^2}{dr^2}+V_L\,, \tag{2.2}$$

and assume that we know the two eigenfunctions of H_0, namely S (the regular solution) and C (the irregular solution).[12] For example, for $V_L=0$,

$S=k^{-1/2}\sin kr$ and $C=k^{-1/2}\cos kr$.

Our variational functional[1] is

$$F_t=\frac{\langle\tilde{C}|V_S|S\rangle\langle S|V_S|\tilde{C}\rangle}{\langle\tilde{C}|\hat{H}-tX|\tilde{C}\rangle}, \tag{2.3}$$

where $\hat{H}=E-H$ and $X=V_S|S\rangle\langle S|V_S$. $\tilde{C}$ is defined by $\Psi-S$, and satisfies

$$\hat{H}|\tilde{C}\rangle=V_S|S\rangle . \tag{2.4}$$

The function $\tilde{C}$ has the form

$$\tilde{C}=\begin{cases}\lambda C, & \text{for } r\geq B\\ \sum a_i v_i, & \textit{for } r\leq B ,\end{cases} \tag{2.5}$$

where λ is the tangent of the phase shift due to V_S. The v_i's are discrete basis functions. If each basis function has the same logarithmic derivative as that of λC, $\tilde{C}$ should be smooth at the boundary. The logarithmic derivative (L_B) of $\tilde{C}$ at the boundary is given by

$$L_B=\frac{\tilde{C}'}{\tilde{C}}\bigg|_{r=B}=\frac{\lambda C'}{\lambda C}\bigg|_{r=B} \tag{2.6}$$

$$=-\tan kB \quad (\text{for } V_L=0). \tag{2.7}$$

Owing to the cancellation[13] of λ in Eq. (2.6), L_B turns out to be a known quantity. With this L_B, one can impose this condition on each v_i. This can be done by writing v_i as

$$v_i=u_i-p_i\bar{u} , \tag{2.8}$$

where the u_i and $\bar{u}$ are arbitrary functions with $u_i(0)=0$ and $\bar{u}(0)=0$ and

$$p_i=\frac{L_B u_i(B)-u_i'(B)}{L_B\bar{u}(B)-\bar{u}'(B)} . \tag{2.9}$$

All the basis functions v_i's hence have the common logarithmic derivative L_B, and so does the interior component of $\tilde{C}$. Thus the wave function $S+\tilde{C}$ is smooth.

The boundary conition for the basis functions v_i in Eq. (2.8) may be stated more generally. As discussed in the previous paper,[1] $\hat{H}$ should be a Hermitian with respect to the basis in which $\tilde{C}$ is expanded. This fact is important, since based on this Hermiticity the stationary property of the variational functional F_t of Eq. (2.3) is ensured. Following Bloch,[14] we rewrite Eq. (2.4) as

$$\tfrac{1}{2}[(\hat{H}+\hat{H}^\dagger)+(\hat{H}-\hat{H}^\dagger)]|\tilde{C}\rangle=V|S\rangle . \tag{2.10}$$

It immediately follows from the above discussion that the matrix element of the anti-Hermitian part is zero for each v_i, namely,

$$\langle v_i|\hat{H}-\hat{H}^\dagger|\tilde{C}\rangle_B=0 . \tag{2.11}$$

Furthermore, since the above integral is a surface one and defining a function C^* by

$$C^*=\begin{cases}C, & \text{at the boundary}\\ 0, & \text{at the origin,}\end{cases} \tag{2.12}$$

we can replace the condition, Eq. (2.11), with

$$\langle v_i|\hat{H}-\hat{H}^\dagger|C^*\rangle_B=0 . \tag{2.13}$$

It is easy to see that the logarithmic derivative condition for the one-dimensional radial function of Eq. (2.1) is a special case of the general condition, since

$$\begin{aligned}\langle v_i|\hat{H}-\hat{H}^\dagger|C^*\rangle&=\frac{1}{2}v_i C\left(\frac{C'}{C}-\frac{v_i'}{v_i}\right)\bigg|_{r=B}\\&=0 ,\end{aligned} \tag{2.14}$$

assuming $C(B)\neq 0$ and $v_i(B)\neq 0$.

The exterior component of $\tilde{C}$ makes no contribution to the functional F_t. Also, since all v_i's have a common logarithmic derivative, $\hat{H}$ in this functional remains Hermitian even within the range of $0\leq r\leq B$. Therefore, variation of F_t gives

$$F_t=\sum_{ij}\langle S|V_s|v_i\rangle_B A_{ij}\langle v_j|V_s|S\rangle_B , \tag{2.15}$$

where

$$(A^{-1})_{ij}=\langle v_i|(\hat{H}-tX)|v_j\rangle_B . \tag{2.16}$$

In the above equations $\langle\ \rangle_B$ means an integration over the range of 0 to B. With this F_t, λ is obtained as[1]

$$\lambda=-2\langle S|V_s|S\rangle-2\frac{F_t}{1+tF_t} . \tag{2.17}$$

As stated in I, the paramenter t can be used to avoid anomalous singularities or to obtain a minimum principle for F_t.

Our variational method developed here does require imposing a boundary condition on the basis functions v_i's. However, various techniques previously developed for the R-matrix theories,[2,10(b)] e.g., procedures for the evaluation of matrix elements, can be applied to our formalism.

III. APPLICATION TO HUCK PROBLEM

To illustrate how our procedure works, we apply it to an exactly soluble two-channel problem proposed by Huck.[15] The total Hamiltonian $H=H_0+V$ is

$$H_0=|\chi_1\rangle\left(-\frac{1}{2}\frac{d^2}{dr^2}\right)\langle\chi_1|+|\chi_2\rangle\left(-\frac{1}{2}\frac{d^2}{dr^2}+\Delta E\right)\langle\chi_2| \tag{3.1}$$

and

$$V=\sum_{m\neq n}^{2}|\chi_m\rangle V_{mn}\langle\chi_n| , \tag{3.2}$$

where

$$V_{12}=V_{21}=\begin{cases}\frac{1}{2}C & (r<B)\\ 0 & (r\geq B),\end{cases} \quad (3.3)$$

$\langle\chi_m|\chi_n\rangle=\delta_{mn}$, and $B=1.0$.

The regular and irregular solutions of H_0 are simply

$$S_m=|\chi_m\rangle k_m^{-1/2}\sin k_m r \quad (3.4a)$$

and

$$C_m=|\chi_m\rangle k_m^{-1/2}\cos k_m r \quad (m=1,2)\,. \quad (3.4b)$$

The logarithmic derivative for each channel is

$$L_B^m=-\tan k_m B \quad (m=1,2). \quad (3.5)$$

On the other hand, the primitive L^2 basis functions u_i^m are

$$u_i^m=|\chi_m\rangle r^i e^{-ar} \quad (i=1,2,\cdots,N)\,. \quad (3.6)$$

To obtain basis functions with a specific logarithmic derivative L_B, we define

$$v_i^m=u_i^m-p_i^m u_{N+1}^m \quad (i=1,2,\cdots,N). \quad (3.7)$$

In Tables I–III, we compare our K-matrix and cross sections with those given by the Schwinger principle[3] as well as by some standard variational methods. They are again the AF,[4] MN,[5] OAF,[6] and RIAF[7] methods. The results in the tables are for the case of $E=0.5$, $\Delta E=0.375$ (so $k_1=1.0$ and $k_2=0.5$), and $C^2=10.0$ [Eq. (3.3)]. In Table I, a comparison of the accuracy for the K matrices is presented. The Schwinger principle still gives the best results and this is due to the fact that the Schwinger principle is based on the integral equation. However, we emphasize that the new method gives results which are significantly better than those of the standard variational methods. For $N=4$, it gives a better K matrix than those of the other standard variational methods with $N=25$. Furthermore, at $N=6$ almost the exact results has already been obtained.

Although the choice of $a=2.5$ for the parameter of the basis functions [Eq. (3.6)] may be optimum for the standard variational methods,[5] it is possible that other a's may be better for this variational method and the Schwinger variational principle. For the Schwinger principle and for the new variational method, the value of $a=0.9$ and $a=0.3$, respectively, are the best. (In general, it is likely that the optimized a's for these two methods should be similar to each other, since both wave functions are expanded over only the range from 0 to B.) The results in Table II show the significant improvement in the convergence. Our fractional functional method with $a=0.3$ gave a better K matrix at $N=3$ than the standard variational

TABLE I. The accuracy of computed K matrices.[a] The deviations from the exact value[b] are shown (ΔK).

		AF[c]	MN[d]	OAF[e]	RIAF[f]	Schwinger[g]	This work
ΔK_{11}	$N=1$		−18.728 53			−19.092 77	−21.075 31
	2		−58.419 20			−0.261 31	−15.193 25
	4	−5.617 43	−5.697 84	−4.548 47		−0.010 00	−0.087 29
	6	−2.997 26	−3.290 61	−2.999 89	−3.004 48	0.0	−0.000 01
	10	−1.391 31	−1.404 72	−1.378 81	−1.390 40	0.0	0.0
	25	−0.363 30		−0.335 32	−0.299 85	0.0	0.0
ΔK_{12}	$N=1$		11.866 03			12.106 30	13.297 24
	2		37.847 36			0.078 61	9.866 51
	4	3.578 88	3.661 93	2.892 39		0.006 00	0.057 55
	6	1.913 96	2.096 20	1.915 79	1.918 39	0.0	0.0
	10	0.889 09	0.897 39	0.881 15	0.888 50	0.0	0.0
	25	0.230 37		0.213 63	0.191 17	0.0	0.0
ΔK_{22}	$N=1$		−7.544 69			−7.579 20	−8.518 01
	2		−24.525 84			0.016 83	−6.415 02
	4	−2.282 98	−2.359 53	−1.843 41		−0.003 55	−0.038 03
	6	−1.223 97	−1.337 19	−1.225 25	−1.226 70	0.0	−0.000 01
	10	−0.568 96	−0.574 10	−0.563 93	−0.568 58	0.0	0.0
	25	−0.146 21		−0.136 19	−0.121 98	0.0	0.0

[a] $a=2.5$.
[b] The exact K matrix[c]; $K_{11}=21.765\,25$, $K_{12}=K_{21}=-14.127\,42$, and $K_{22}=8.733\,85$.
[c] References 4 and 6.
[d] Reference 5.
[e] Reference 6.
[f] Reference 7.
[g] Reference 3.

TABLE II. The accuracy of the K matrices with optimized values of the exponents in Eq. (3.6).

N		ΔK_{11} Schwinger	ΔK_{11} This work	ΔK_{12} Schwinger	ΔK_{12} This work	ΔK_{22} Schwinger	ΔK_{22} This work
$a=0.3$	1	−8.858 57	−14.847 69	5.562 03	9.477 45	−3.485 26	−6.072 02
	2	−1.006 88	−0.341 69	0.635 20	0.218 64	−0.400 53	−0.140 17
	3	−0.002 21	−0.024 06	0.001 39	0.015 30	−0.000 88	−0.009 73
	4	−0.000 18	0.0	0.000 11	0.0	−0.000 08	−0.000 01
	5	0.0	0.0	0.0	0.0	0.0	0.0
$a=0.9$	1	−0.142 59	−18.952 90	−0.091 41	12.089 00	0.194 92	−7.761 97
	2	−1.539 71	−1.530 49	0.965 67	0.996 16	−0.604 78	−0.650 41
	3	−0.015 96	−0.015 34	0.009 90	0.010 10	−0.006 12	−0.006 71
	4	−0.000 04	−0.000 73	0.000 02	0.000 46	−0.000 02	0.0
	5	0.0	0.0	0.0	0.0	−0.000 01	0.0

methods of $N=25$. At $N=4$, it is almost completely converged.

In Table III, the deviation of computed cross sections from the exact values are tabulated. The cross sections are much less sensitive than the K matrices are.[3] In spite of this, our fractional variational method and the Schwinger variational principle give far better cross sections than the standard variational methods. We can conclude that our new method is quite promising.

IV. DISCUSSION

As shown numerically in Sec. III, the convergence of our method is remarkably better than that of the standard variational methods. In this section, we will discuss some factors which reduce the rate of convergence of the standard variational principles, especially in connection with the Huck problem.

In the standard variational methods, the wave function of mth channel has the form over the entire range,

$$\Psi_m = S_m + \sum_n \overline{C}_n K_{nm} + \sum_{in} d_{in}^m u_i^n \,, \tag{4.1}$$

where $\overline{C}_m$ coincides with C_m in the asymptotic region and is regular at the origin. In the Huck

TABLE III. The convergence of the approximate cross sections. The deviations from the exact values [a] are presented.

N		AF[b,d]	MN[c,d]	Schwinger[e]	This work[f]
ΔQ_{11}	1	−0.271 29	−0.264 26	−0.041 45	−0.043 33
	2	−0.013 87	−0.013 36	−0.005 16	−0.000 11
	3	−0.049 53	−0.025 50	0.000 49	−0.000 03
	4	−0.008 07	0.000 68	0.0	0.0
ΔQ_{12}	1	0.085 84	0.080 55	0.013 42	0.022 54
	2	0.005 17	−0.012 68	0.002 15	0.000 14
	3	0.006 65	0.013 99	0.000 03	0.000 02
	4	0.004 75	0.002 00	0.0	0.0
ΔQ_{21}	1	0.343 34	0.322 20	0.053 66	0.090 15
	2	0.020 68	−0.050 74	0.008 60	0.000 64
	3	0.026 59	0.055 96	0.000 11	0.000 07
	4	0.018 99	0.008 00	0.0	0.0
ΔQ_{22}	1	0.004 54	−0.122 61	−0.044 18	−0.018 09
	2	0.036 00	0.188 66	−0.002 62	0.000 35
	3	0.160 17	−0.025 10	−0.000 05	−0.000 03
	4	−0.002 19	0.003 04	−0.000 01	0.0

[a]The exact cross sections (Ref. 4); $Q_{11}=2.167\,91$, $Q_{12}=0.767\,46$, $Q_{21}=3.069\,85$, and $Q_{22}=2.558\,44$.
[b]Reference 6.
[c]Reference 5.
[d]$a=2.5$.
[e]$a=0.9$, Ref. 3.
[f]$a=0.3$.

model, $\overline{C}_m$ is chosen to be[4–7]

$$\overline{C}_m = |\chi_m\rangle k^{-1/2} (1-e^{-r}) \cos k_m r. \quad (4.2)$$

Therefore the matrix elements which are necessary for the standard variational methods are

$$\langle u_i^m|\hat{H}|u_j^n\rangle, \langle u_i^m|\hat{H}|S_n\rangle, \langle u_i^m|\hat{H}|\overline{C}_n\rangle,$$
$$\langle S_m|\hat{H}|S_n\rangle, \langle S_m|\hat{H}|\overline{C}_n\rangle,$$

and

$$\langle \overline{C}_m|\hat{H}|\overline{C}_n\rangle .$$

On the other hand, only

$$\langle u_i^m|\hat{H}|u_j^n\rangle_B, \langle u_i^m|V|S_n\rangle_B,$$

and

$$\langle S_m|V|S_n\rangle_B$$

are necessary for our method. We do not need any integrals involving the $\overline{C}_m$ functions. This is convenient, since the integrals involving $\overline{C}_m$ are cumbersome in general.

It can be easily seen that the form of $\overline{C}_m$, Eq. (4.2), tends to reduce the convergence of the variational calculations. It is desirable that beyond the point B (in the exterior region), $\overline{C}_m$ should coincide with C_m itself, since $\hat{H}$ is equal to $\hat{H}_0$ there. However, $\overline{C}_m$ of Eq. (4.2) cannot meet this condition. Oberoi and Nesbet[16] proposed the numerical asymptotic function (NAF) method, in which $\overline{C}_m$ can have exactly the same form as C_m in the exterior region via numerical integration. They choose

$$(E-H_0)\overline{C}_m = 0 \quad (\overline{C}_m = C_m) \quad r \geq B \quad (4.3a)$$

$$\overline{C}_m = a_1^n g_1 + a_2^n g_2 \quad 0 \leq r \leq B , \quad (4.3b)$$

where the functions g_1 and g_2 are arbitrary and the coefficients a_1 and a_2 are determined so that $\overline{C}_m$ behaves regularly at the origin and is smooth at $r=B$.[17] By this replacement, the standard variational principles can take some advantage of the R-matrix method but still retains the smoothness of the wave function, and, of course, can show better convergence.[16] The calculations with the NAF method suggest[16] that the results depend on the selection of g_1 and g_2, even if the same short-range functions are used. Again, we will stress that $\overline{C}_m$'s do not appear in our formalism explicity, although the exact C_m functions are used in the exterior region[12] as well as in the NAF method.

Another factor which reduces the convergence of the standard variational methods comes from the L^2 functions in Eq. (4.1). In the exterior region, Ψ must be expressed exclusively by the linear combination of only S_m and C_m $(m=1,2,\cdots)$. So, one needs extra short-range functions there to cancel out the tail of the functions $\sum_{i,n} d_{in}^m u_i^n$ [see Eq. (4.1)] which penetrate into the exterior region. Therefore, unless all u_i^n die off within the boundary B, the L^2 functions themselves can hurt the convergence rate. In this sense, even the NAF method is still unsatisfactory, since L^2 functions are defined throughout the whole space. In contrast, in our formalism [see Eq. (2.5)] the L^2 functions are truncated up to the boundary B and used to expand only the interior component of Ψ. Therefore, by this extension of the definition of the basis functions, which was naturally introduced by our fractional functional, we can expect a faster convergence over the NAF method and, of course, over the standard variational methods.

V. CONCLUDING REMARKS

We have proposed a new variational principle which is based on a functional of fractional form. The method is similar to the R-matrix theory in the sense that the configuration space is divided into two parts. The resultant wave function is smooth everywhere. This is important since the lack of smoothness of the wave function at the boundary can result in a slow convergence in some R-matrix methods.[11] It may be again emphasized that our resultant K matrix[1] is symmetric (the S matrix is unitary) and variationally stable. It is also free from singularities.

The results of the application to the model problem are very encouraging and have shown our new approach is much superior to the other standard variational principles. We note that the Schwinger variational principle gives very accurate results and seems to be more stable with regard to changes of basis functions. We must note also that the Schwinger variational principle does not require any artificial boundary. However, we find that with a good basis set our new method can be as accurate as the Schwinger principle. This is important since the computational requirements of our new method are less than those of the Schwinger principle which requires the double integration associated with the Green's function. In addition, one can find good basis sets for our method using the minimum principle stated earlier.[1]

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